Berry's phases and topological properties in the Born-Oppenheimer approximation[1]

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Abstract

The level crossing problem is neatly formulated by the second quantized formulation, which exhibits a hidden local gauge symmetry. The analysis of geometric phases is reduced to a simple diagonalization of the Hamiltonian. If one diagonalizes the geometric terms in the infinitesimal neighborhood of level crossing, the geometric phases become trivial (and thus no monopole singularity) for arbitrarily large but finite time interval T. The topological proof of the Longuet-Higgins' phase-change rule, for example, thus fails in the practical Born-Oppenheimer approximation where T is identified with the period of the slower system. The crucial difference between the Aharonov-Bohm phase and the geometric phase is explained. It is also noted that the gauge symmetries involved in the adiabatic and non-adiabatic geometric phases are quite different.

1 Introduction

The geometric phases revealed the importance of hitherto un-recognized phase factors in the adiabatic approximation[1, 2, 3, 4, 5, 6]. It may then be interesting to investigate how those phases behave in the exact formulation. We formulate the level crossing problem by using the second quantization technique, which works both in the path integral and operator formulations[7, 8, 9]. In this formulation, the analysis of geometric phases is reduced to the familiar diagonalization of the Hamiltonian. Also, a hidden local gauge symmetry replaces the notions of parallel transport and holonomy.

When one diagonalizes the Hamiltonian in a very specific limit, one recovers the conventional geometric phases defined in the adiabatic approximation. If one diagonalizes the Hamiltonian in the other extreme limit, namely, in the infinitesimal neighborhood of level crossing for any fixed finite time interval T, one can show that the geometric phases become trivial and thus no monopole-like singularity. At the level crossing point, the conventional energy eigenvalues become degenerate but the degeneracy is lifted if one diagonalizes the geometric terms. Our analysis shows that the topological interpretation[3, 1] of geometric phases such as the topological proof of the Longuet-Higgins' phase-change rule[4] fails in the practical Born-Oppenheimer approximation where T is identified with

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the period of the slower system. This analysis shows that the topological properties of the geometric phase and the Aharonov-Bohm phase are quite different.

Also, the difference between gauge symmetries for adiabatic phase and "non-adiabatic phase" by Aharonov-Anandan[10] becomes quite clear in this formulation.

2 Second quantized formulation

We start with the generic hermitian Hamiltonian $\hat{H} = \hat{H}(\hat{\vec{p}}, \hat{\vec{x}}, X(t))$ for a single particle theory in a slowly varying background variable $X(t) = (X_1(t), X_2(t), ...)$. The path integral for this theory for the time interval $0 \leq t \leq T$, which is taken to be the period of the slower background system, in the second quantized formulation is given by

$$\int \mathcal{D}\psi^\star \mathcal{D}\psi \exp\{\frac{i}{\hbar}\int_0^T dt d^3x[\mathcal{L}]\}$$

where

$$\mathcal{L} = \psi^\star(t,\vec{x}) i\hbar\frac{\partial}{\partial t}\psi(t,\vec{x}) - \psi^\star(t,\vec{x})\hat{H}(\frac{\hbar}{i}\frac{\partial}{\partial\vec{x}}, \vec{x}, X(t))\psi(t,\vec{x}). \quad (1)$$

We then define a complete set of eigenfunctions

$$\begin{aligned} &\hat{H}(\frac{\hbar}{i}\frac{\partial}{\partial\vec{x}}, \vec{x}, X(t)) v_n(\vec{x}, X(t)) = \mathcal{E}_n(X(t)) v_n(\vec{x}, X(t)), \\ &\int d^3x v_n^\star(\vec{x}, X(t)) v_m(\vec{x}, X(t)) = \delta_{n,m} \end{aligned} \quad (2)$$

and expand

$$\psi(t,\vec{x}) = \sum_n b_n(t) v_n(\vec{x}, X(0)). \quad (3)$$

The path integral for the time interval $0 \leq t \leq T$ in the second quantized formulation is given by

$$\begin{aligned} Z = &\int \prod_n \mathcal{D}b_n^\star \mathcal{D}b_n \exp\{\frac{i}{\hbar}\int_0^T dt[\sum_n b_n^\star(t) i\hbar\frac{\partial}{\partial t}b_n(t) \\ &+ \sum_{n,m} b_n^\star(t)\langle n|i\hbar\frac{\partial}{\partial t}|m\rangle b_m(t) - \sum_n b_n^\star(t)\mathcal{E}_n(X(t))b_n(t)]\} \end{aligned} \quad (4)$$

where the second term in the action stands for the term commonly referred to as Berry's phase[1] and its off-diagonal generalization. The second term is defined by

$$\langle n|i\hbar\frac{\partial}{\partial t}|m\rangle \equiv \int d^3x v_n^\star(\vec{x}, X(t)) i\hbar\frac{\partial}{\partial t} v_m(\vec{x}, X(t)). \quad (5)$$

In the operator formulation of the second quantized theory, we thus obtain the effective Hamiltonian

$$\hat{H}_{eff}(t) \;=\; \sum_n \hat{b}_n^\dagger(t)\mathcal{E}_n(X(t))\hat{b}_n(t) - \sum_{n,m} \hat{b}_n^\dagger(t)\langle n|i\hbar\frac{\partial}{\partial t}|m\rangle \hat{b}_m(t). \tag{6}$$

When we define the Schrödinger picture $\hat{\mathcal{H}}_{eff}(t)$ by replacing all $\hat{b}_n(t) \to \hat{b}_n(0)$ in $\hat{H}_{eff}(t)$ we can show[7, 8]

$$\langle n(T)|T^\star \exp\{-\frac{i}{\hbar}\int_0^T \hat{H}(\hat{\vec{p}}, \hat{\vec{x}}, X(t))dt\}|n(0)\rangle = \langle n|T^\star \exp\{-\frac{i}{\hbar}\int_0^T \hat{\mathcal{H}}_{eff}(t)dt\}|n\rangle. \tag{7}$$

Both-hand sides of this formula are exact, but the difference is that the geometric terms, both of diagonal and off-diagonal, are explicit in the second quantized formulation on the right-hand side. The state vectors in the second quantization are defined by $|n\rangle = \hat{b}_n^\dagger(0)|0\rangle$, and the state vectors in the first quantized states by (2). If one retains only the diagonal elements in this formula (7), one recovers the conventional adiabatic formula[5]

$$\exp\{-\frac{i}{\hbar}\int_0^T dt[\mathcal{E}_n(X(t)) - \langle n|i\hbar\frac{\partial}{\partial t}|n\rangle]\}. \tag{8}$$

The above formula (7) represents the essence of geometric phases: If one performs an exact evaluation one does not obtain a clear physical picture of what is going on. On the other hand, if one makes an adiabatic approximation one obtains a clear universal picture.

The path integral formula (4) is based on the expansion (3), and the starting theory depends only on the field variable $\psi(t, \vec{x})$, not on $\{b_n(t)\}$ and $\{v_n(\vec{x}, X(t))\}$ separately. This fact shows that our formulation contains a hidden local gauge symmetry

$$\begin{aligned} &v_n'(\vec{x}, X(t)) = e^{i\alpha_n(t)} v_n(\vec{x}, X(t)), \\ &b_n'(t) = e^{-i\alpha_n(t)} b_n(t) \end{aligned} \tag{9}$$

where the gauge parameter $\alpha_n(t)$ is a general function of t. By using this gauge freedom, one can choose the phase convention of the basis set $\{v_n(\vec{x}, X(t))\}$ at one's will such that the analysis of geometric phases becomes simplest. From the view point of hidden local symmetry, the formula (8) is a result of the specific choice of eigenfunctions $v_n(\vec{x}, X(0)) = v_n(\vec{x}, X(T))$ in the gauge invariant expression

$$v_n(\vec{x}; X(0))^\star v_n(\vec{x}; X(T)) \exp\{-\frac{i}{\hbar}\int_0^T [\mathcal{E}_n(X(t)) - \langle n|i\hbar\frac{\partial}{\partial t}|n\rangle]dt\}. \tag{10}$$

This hidden local symmetry replaces the notions of paralell transport and holonomy in the analyses of geometric phases, and it works not only for cyclic but also for non-cyclic evolutions[9].

3 Level crossing problem

For a simplified two-level problem, the Hamiltonian is defined by the matrix in the neighborhood of level crossing [7]

$$h(X(t)) = \begin{pmatrix} E(t) & 0 \\ 0 & E(t) \end{pmatrix} + g\sigma^l y_l(t) \tag{11}$$

after a suitable re-definition of the parameters by taking linear combinations of $X_k(t)$. Here $y_l(t)$ stands for the background variable and σ^l for the Pauli matrices, and g is a suitable (positive) coupling constant.

The eigenfunctions in the present case are given by

$$v_+(y) = \begin{pmatrix} \cos\frac{\theta}{2}e^{-i\varphi} \\ \sin\frac{\theta}{2} \end{pmatrix}, \quad v_-(y) = \begin{pmatrix} \sin\frac{\theta}{2}e^{-i\varphi} \\ -\cos\frac{\theta}{2} \end{pmatrix} \tag{12}$$

by using the polar coordinates, $y_1 = r\sin\theta\cos\varphi,\ y_2 = r\sin\theta\sin\varphi,\ y_3 = r\cos\theta$. Note that, by using hidden local symmetry, our eigenfunctions are chosen to be periodic under a 2π rotation around 3-axis, which is quite different from a 2π rotation of a spin-1/2 wave function. If one defines

$$v_m^\dagger(y)i\frac{\partial}{\partial t}v_n(y) = A^k_{mn}(y)\dot{y}_k$$

where m and n run over $\pm$, we have

$$\begin{aligned} A^k_{++}(y)\dot{y}_k &= \frac{(1+\cos\theta)}{2}\dot{\varphi} \\ A^k_{+-}(y)\dot{y}_k &= \frac{\sin\theta}{2}\dot{\varphi} + \frac{i}{2}\dot{\theta} = (A^k_{-+}(y)\dot{y}_k)^\star, \\ A^k_{--}(y)\dot{y}_k &= \frac{1-\cos\theta}{2}\dot{\varphi}. \end{aligned} \tag{13}$$

The effective Hamiltonian (6) is then given by

$$\hat{H}_{eff}(t) = (E(t)+gr(t))\hat{b}^\dagger_+\hat{b}_+ + (E(t)-gr(t))\hat{b}^\dagger_-\hat{b}_- - \hbar\sum_{m,n}\hat{b}^\dagger_m A^k_{mn}(y)\dot{y}_k\hat{b}_n. \tag{14}$$

with $r(t) = \sqrt{y_1^2+y_2^2+y_3^2}$. The point $r(t)=0$ corresponds to the level crossing. In the adiabatic approximation, one neglects the off-diagonal terms in the last geometric terms, which is justified for $Tgr(t) \gg \hbar\pi$, where $\hbar\pi$ stands for the magnitude of the geometric term times T. The adiabatic formula (8) then gives the familiar result

$$\exp\{i\pi(1-\cos\theta)\} \times \exp\{-\frac{i}{\hbar}\int_{C(0\rightarrow T)} dt[E(t)-gr(t)]\} \tag{15}$$

for a 2π rotation in φ with fixed θ, for example.

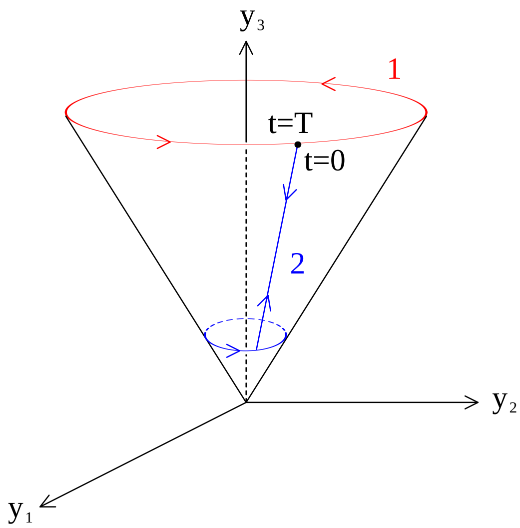

Fig. 1: The path 1 gives the conventional geometric phase for a fixed finite T, whereas the path 2 gives a trivial geometric phase for a fixed finite T. Note that both of the paths cover the same solid angle $2\pi(1-\cos\theta)$.

To analyze the behavior near the level crossing point, we perform a unitary transformation $\hat{b}_m = \sum_n U(\theta(t))_{mn}\hat{c}_n$ where m,n run over $\pm$ with

$$U(\theta(t)) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}, \tag{16}$$

which diagonalizes the geometric terms and the above effective Hamiltonian (13) is written as

$$\hat{H}_{eff}(t) \simeq (E(t)+gr\cos\theta)\hat{c}_+^\dagger\hat{c}_+ + (E(t)-gr\cos\theta)\hat{c}_-^\dagger\hat{c}_- - \hbar\dot{\varphi}\hat{c}_+^\dagger\hat{c}_+ \tag{17}$$

in the infinitesimal neighborhood of the level crossing point, namely, for sufficiently close to the origin of the parameter space $(y_1(t), y_2(t), y_3(t))$ but $(y_1(t), y_2(t), y_3(t)) \neq (0,0,0)$. To be precise, for any given *fixed* time interval T, we can choose in the infinitesimal neighborhood of level crossing $Tgr(t) \ll T\hbar\dot{\varphi} \sim 2\pi\hbar$. In this new basis, the geometric phase appears only for the mode $\hat{c}_+$ which gives rise to a phase factor

$$\exp\{i\int_C \dot{\varphi}dt\} = \exp\{2i\pi\} = 1, \tag{18}$$

and thus no physical effects. In the infinitesimal neighborhood of level crossing, the states spanned by $(\hat{b}_+, \hat{b}_-)$ are transformed to a linear combination of the states spanned by $(\hat{c}_+, \hat{c}_-)$, which give no non-trivial geometric phase.

We emphasize that this topological property is quite different from the familiar Aharonov-Bohm effect [10], which is topologically exact for any finite time interval T. Besides, the setting of the Aharonov-Bohm effect differs from the present level crossing problem in the fact that the space is not simply connected in the case of the Aharonov-Bohm effect.

4 Non-adiabatic phase

We comment that the non-adiabatic phase by Aharonov and Anandan [10] is based on the equivalence class (or gauge symmetry) which identifies all the Schrödinger amplitudes of the form

$$\{e^{i\alpha(t)}\psi(t,\vec{x})\}. \tag{19}$$

This gauge symmetry is quite different from our hidden local symmetry which is related to an arbitrariness of the choice of coordinates in the functional space.

5 Discussion

The notion of Berry's phase is known to be useful in various physical contexts[11]. Our analysis however shows that the topological interpretation of Berry's phase associated with level crossing generally fails in the practical Born-Oppenheimer approximation where T is identified with the period of the slower system. The notion of "approximate topology" has no rigorous meaning, and it is important to keep this approximate topological property of geometric phases associated with level crossing in mind when one applies the notion of geometric phases to concrete physical processes.

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